Agilent

Agilent NGA RGA

User Guide

Notices

Edition

Second edition, June 2021
First edition, September 2015

Printed in USA

Agilent Technologies, Inc.
2850 Centerville Road
Wilmington, DE 19808-1610 USA

Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

Technology Licenses

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

Restricted Rights Legend

If software is for use in the performance of a U.S. Government prime contract or subcontract, Software is delivered and licensed as "Commercial computer software" as defined in DFAR 252.227-7014 (June 1995), or as a "commercial item" as defined in FAR 2.101(a) or as "Restricted computer software" as defined in FAR 52.227-19 (June 1987) or any equivalent agency regulation or contract clause. Use, duplication or disclosure of Software is subject to Agilent Technologies' standard commercial license terms, and non-DOD Departments and Agencies of the U.S. Government will receive no greater than Restricted Rights as defined in FAR 52.227-19(c)(1-2) (June 1987). U.S. Government users will receive no greater than Limited Rights as defined in FAR 52.227-14 (June 1987) or DFAR 252.227-7015 (b)(2) (November 1995), as applicable in any technical data.

Safety Notices

CAUTION

A CAUTION notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a CAUTION notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

Contents

1 Introduction

The analysis of natural gas by gas chromatography is used to estimate the energy content of the natural gas. This provides a means to monitor custody transfer of the natural gas from the producer to the end user. Several organizations (GPA - Gas Processors Association [now in conjunction with the American Petroleum Institute], ASTM international - formally American Society of Testing and Materials, ISO - International Organization for Standardization [which is also considered as DIN standard and other Natural Gas Standards are based on the ISO standards]) have developed standards based on the individual compound energy values and other physical constants. The calculation is based on the assumption that the Natural Gas mixture can be separated into the individual components. This assumption is based on Dalton's law (the total pressure of a gas mixture is the sum of the partial pressures):

$$P = \Sigma\, p_i$$

where pi is the partial pressure on compound i.

When Dalton's law is combined with the ideal gas law:

$$P \times V = n \times R \times T$$

where P is the pressure, V is the volume, T is the temperature and R is the Gas Constant (the value will depend upon the units used for V, T, and P) and n is the number of moles.

When the Temperature and Volume are defined and constant, the number of moles for each component will be proportional to the partial pressure.

$$x_i = p_i/P = n_i/n_{tot}$$

The amount x_i can be calculated from the response of the individual component in the GC separation of the gas mixture. With gas mixtures, the total concentration is normalized to 100 %. The gas mixture suppliers usually provide the gas mixture with concentrations in mole %, however, it is possible that the concentrations will be given in volume % or weight %. If this is the case the volume % or weight % values will need to be converted to mole %, since the values in the tables are given in units/mole.

This requires the ability to execute a series of calculations based on several compound specific physical constants, such as:

- Heating values
- Compressibility factor
- Molecular weight
- Liquid density

OpenLab 2.6 CDS has added features to Data Analysis and enhancements to Reporting that have it made possible to make this calculations. Data Analysis (DA) now provides a Custom Calculator Editor which allows the user to setup custom calculations. Once the custom calculation is executed on the injection results, the results are provided in the Injection Results Table and are available for reports. Reporting now provides a means to link the custom calculation results to the report.

One type of analysis where these features are very useful is in gas analysis. The different standards, such as GPA 2172, ASTM D3588, and ISO 6976, detail the calculation and provide the physical constants necessary to calculate the energy content from the composition determined by Gas Chromatographic analysis. The calculation can be divided into two groups; one being based on English units, Foot Pound Second (FPS) with the energy content being

primarily reported in British Thermal Unit (BTUs) and the other on Metric units with energy content reported in kilo Joule (kJ) or Wobbe Index. When the ISO 6976:2016 Standard was published there were substantial changes that require the addition of a third choice - ISO 6976:2016. The custom calculation file can be linked to a table of the compound specific physical constants which are needed for the different calculations. The Natural Gas Analysis/Refinery Gas Analysis (NGA/RGA) Add-on is a tool to aid the user in the setup of the calculations and the reporting. Once the user makes the selection of which method to update and of the parameters to calculate, the NGA/RGA Add-on will then generate a file to be used for the custom calculations selected, a constants file appropriate to the selection and a report template using the custom calculations selected. When the method is updated it will now have path added for the custom calculation file and a path for the report template. Once the report template is setup, it can be further modified using DA's Reporting tools.

2 DA Method Setup

OpenLab 2.6 can be installed as a standalone workstation or as a client server system. When an instrument is setup, it is required to be associated with at least one Project. The Project is organized as follows:

- Project
  - Analysis template
  - Method
  - Report template
  - Result

The NGA RGA Add-on will update the selected method and save the constants file as a .txt file and the custom calculation file as a .ccf file in the Method folder. It also saves a report template as an .rdl file in the **Report Template** folder. Since this happens at the Project level, these updates are available to be used by any client in a client server that access the method and associated files. This means for a client server system it is only necessary to select one client to install the Add-on.

When setting up your DA method, NGA-RGA Add-on expects some requirements to be fulfilled. If the following requirements are not met, the Add-on will not work as expected.

- The method needs to be set up as a **GC/LC Quantitative** method. This is necessary for the Custom Calculator.

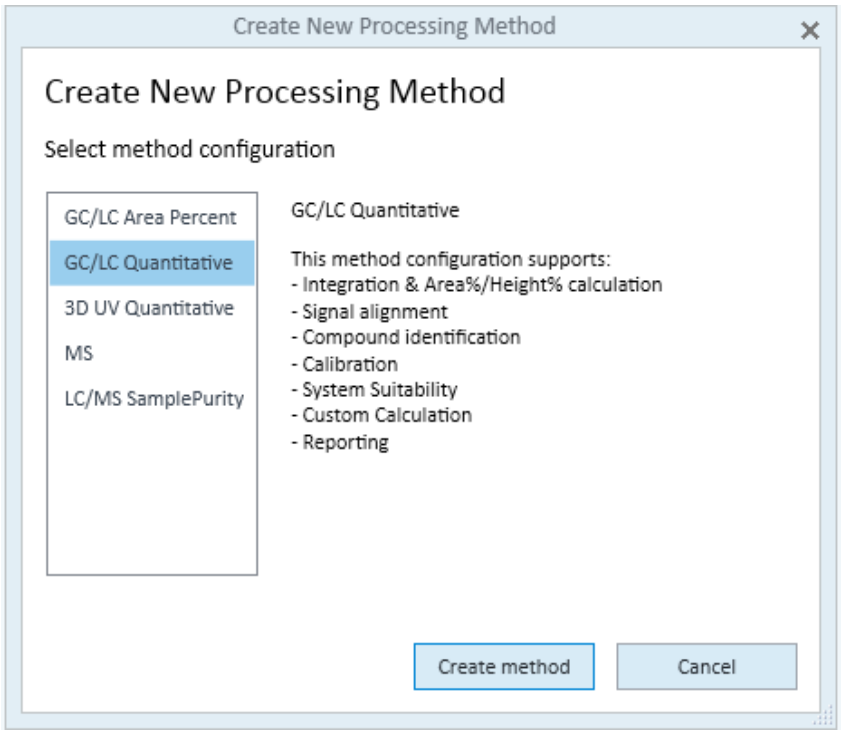


Figure 1. GC/LC Quantitative method

- Compounds must have the exact names as the ones in the constants file, and are case sensitive. See **Appendix A** starting on **page 27** for the list of compounds used with FPS and Metric choices and **Appendix B** starting on **page 33** for the list of compounds used with ISO 6976:2016 selection.
- Calibration in DA must be setup so that the **Amount** value computed by quantification represents the weight %/mol %/volume % according to the calibration type chosen in the Add-on.
- If you need air correction, oxygen and nitrogen compounds must be defined, these are case sensitive.

3 User Workflow

Updating a Data Analysis Method

1 Open Data Analysis from either the Control Panel or Data Acquisition.

- From the Control Panel, select the Project with the data to be used for the calculations and click **Start Data Analysis**. If you have created a Desktop Shortcut, this will also start from the Control Panel.

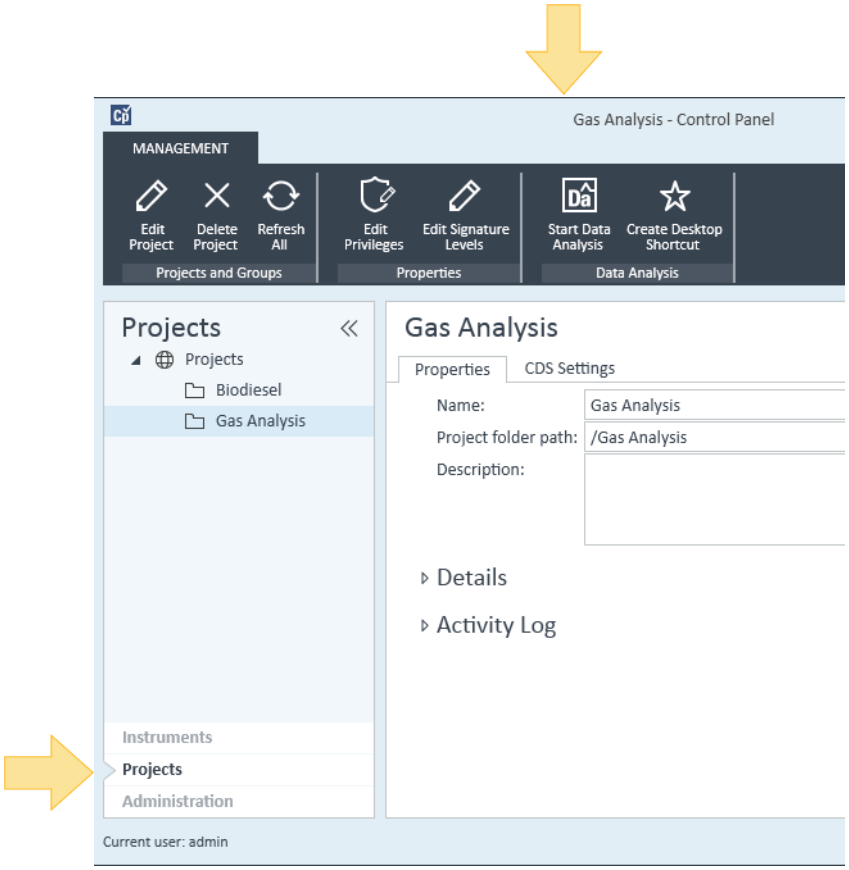


Figure 2. Start Data Analysis

- From Data Acquisition, select the sample in the **Run Queue**, right-click to bring up the choices, and select either of the last two choices, **Review Selected Run in Data Analysis** or **Launch Data Analysis With Current Project**.

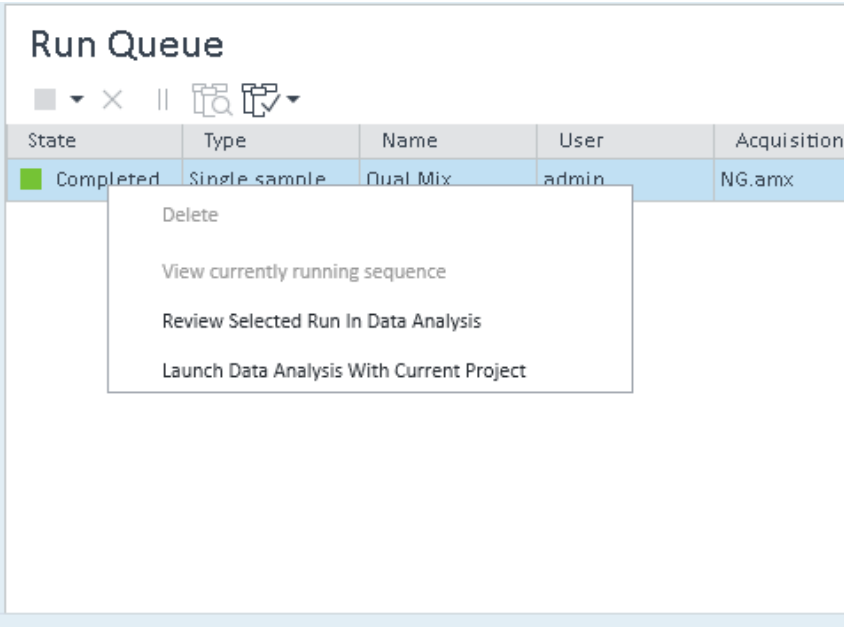


Figure 3. Run Queue

After you select the data file to be loaded, either from the **Run Queue** or from **Data Analysis**, Data Processing will be displayed.

2 Click **NGA RGA** in the **Home** ribbon of Data Processing view.

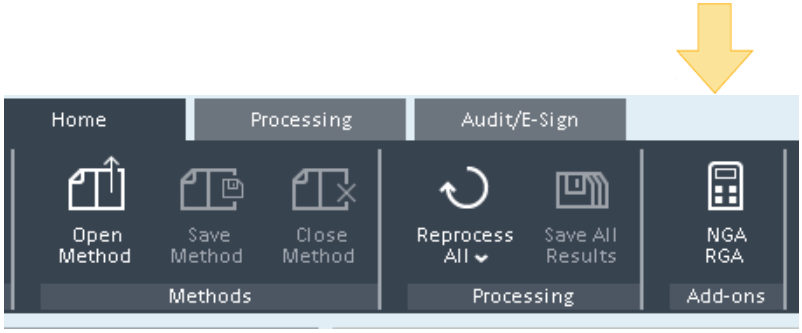


Figure 4. NGA RGA

3 In the **NGA RGA** Add-on window click **Select method** and select the method in the methods folder for the project.

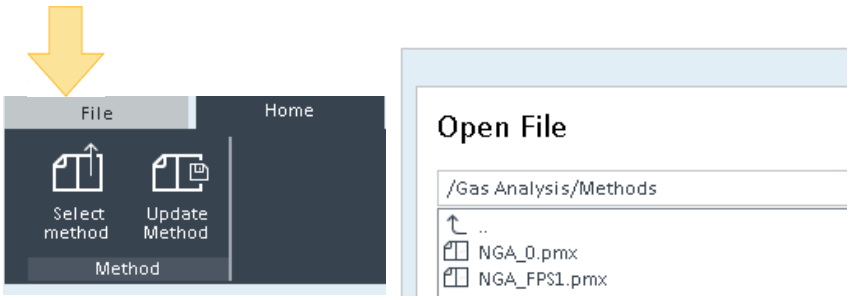


Figure 5. Select Method

4 Select the **Computation type** you want to use (**Metric** or **FPS** or **ISO 6976:2016**).

- **FPS** will provide calculations and constants consistent with GPA and ASTM standards using FPS units (also called English or Engineering).
- **Metric** will provide calculations and constants file consistent with ISO and other European standards.
- **ISO 6976:2016** will provide calculations and constants files consistent with the updates in ISO 6976:2016 based standards.

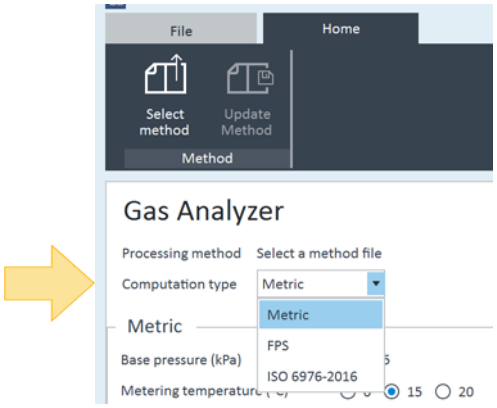


Figure 6. Computation type

5 The **Calibration type** is **Mole %** by default. Change the **Calibration type** to **Volume %** if your calibration table is in volume % or to **Weight %** if your calibration is in weight %.

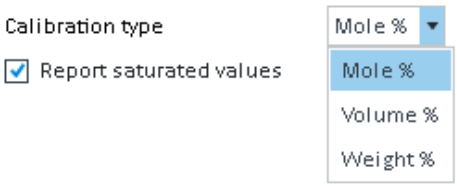


Figure 7. Calibration type

6 Select the other parameters you want to use. For Metric, the metering and combustion temperatures can be selected. Combustion temperatures equal to or greater than the metering temperature can be selected.

7 Click **Update Method** to update your method. A pop up window will confirm that your method has been successfully updated.

If you choose to update your master method then your result set method will not be updated. So you will need to relink the result set with your master method. Be sure to close and reopen your method to see the changes.

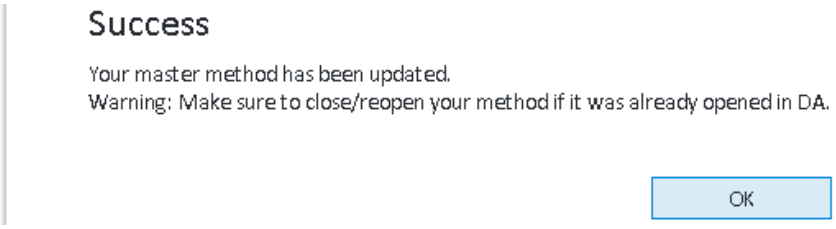


Figure 8. Method updated confirmation

8 Open the method you have updated and link it to your injections.

NOTE **You can see that the Custom Calculation file has been linked to the method. Embedded files are discussed in the OpenLab CDS 2 Help.**

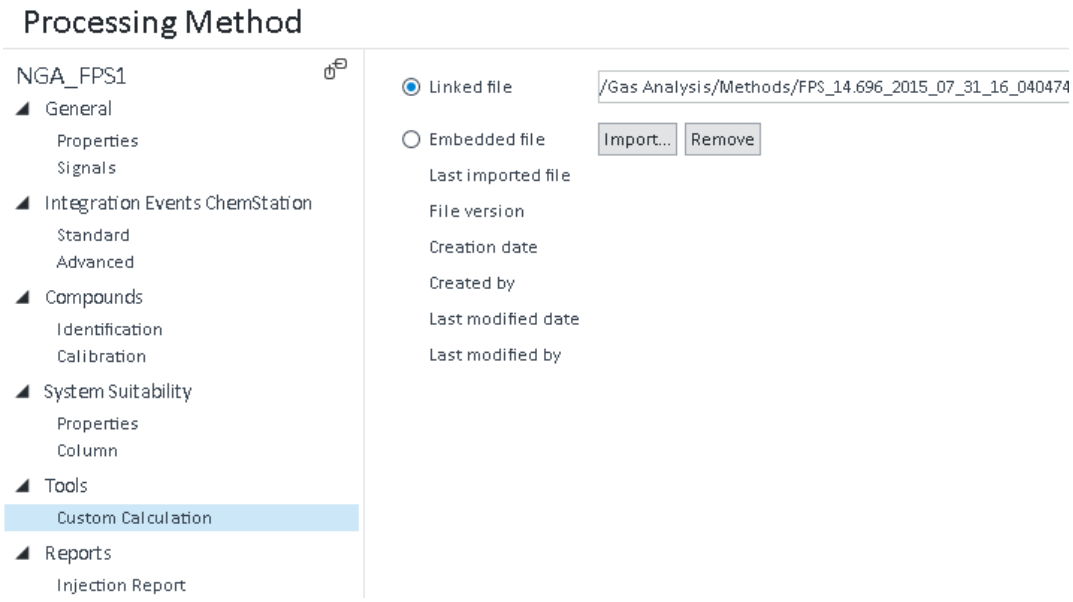


Figure 9. Linked file method

The report template has been updated.

9 Choose the **Report destination** and **File format** to have the report generated. The report can also be copied to the Windows File System by selecting **Windows file system** radio button

in the **Copy report to folder** section. This will allow access to the reports from Windows File Explorer and not require accessing the report in OpenLab Data Store.

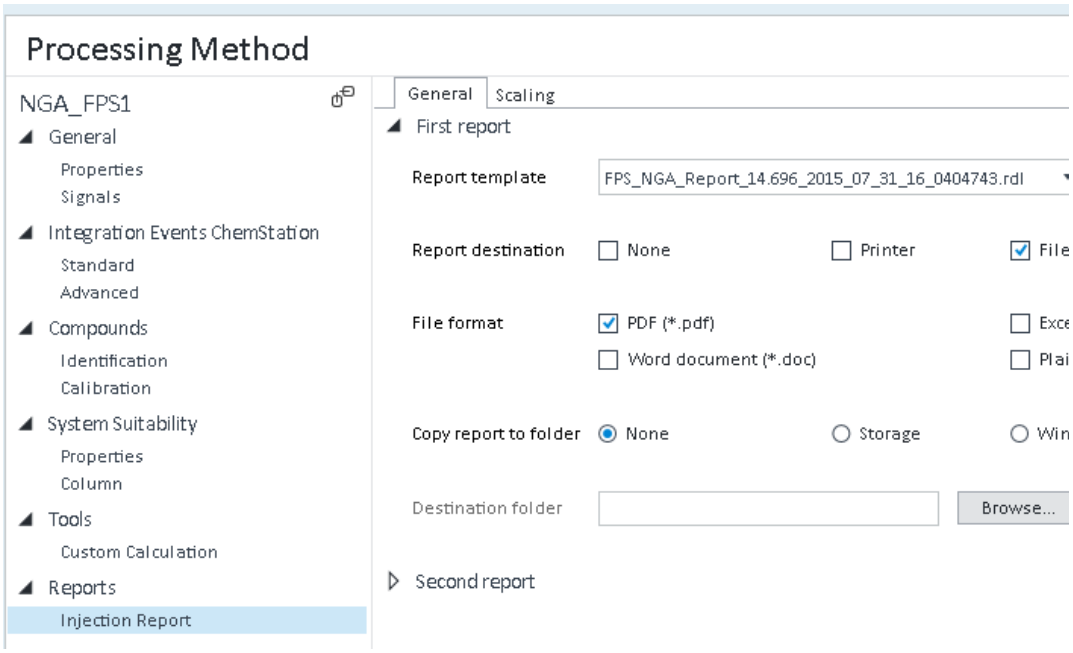


Figure 10. Report file destination

Now the method is ready to use. When this processing method is used, it will execute the custom calculation selected and generate the reports selected after the sample has completed. The NGA RGA Add-on is only used for setup and is not required to run the samples.

Changing a Default Report Template Used During Method Update

The NGA RGA Add-on default templates (FPS_NGA_Report.rdl, Metric_NGA_Report.rdl, and ISO_6976_2016_NGA_Report.rdl) that are used when **Update Method** is selected, are intended to be a starting point.

When you have a modified template, and want to replace the default template used during method update, copy the template to the **Bin** directory of your DA installation (by default it is: C:\Program Files (x86)\Agilent Technologies\OpenLab Data Analysis\Bin).

To get a version of these files, you can use the web browser interface of your OpenLab Data Store to download them. In the OpenLab Data Store they will be stored in the report template folder of your project and named similar to the following example: Metric_NGA_MoleOnlyReport_15_15_2015_02_03_17_2225276.rdl

The names of the reports have to be exact:

- FPS_NGA_Report.rdl (to replace the report used for FPS computation)
- Metric_NGA_Report.rdl (to replace the report used in metric computation)
- ISO_6976_2016_NGA_Report.rdl (to replace the report used for ISO 6976:2016 Computation)

If you need to restore the original template, rename or remove the template from the Bin directory. When this is done, the Add-on will use the embedded template.

The Report template has been set up to contain the values calculated by the custom calculator. The idea was to provide the calculations in the report and for you to modify the report as necessary. The report template can be modified and saved under a new report template name in the Project.

As an example, the label for **Compressibility Factor** can be changed to the Spanish term, **Factor de compresibilidad** by completing the following steps.

1 In Data Analysis, select **Reporting**.

2 Select the **Report Editor** and double-click on the template to be modified.

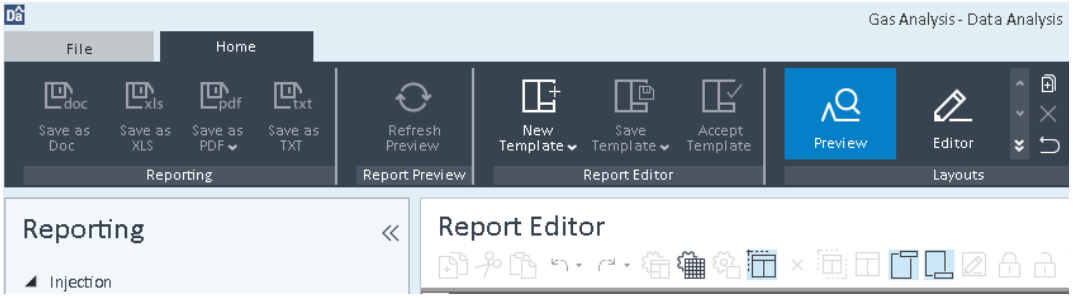


Figure 11. Report Editor

3 Click **Compressibility Factor** to select it.

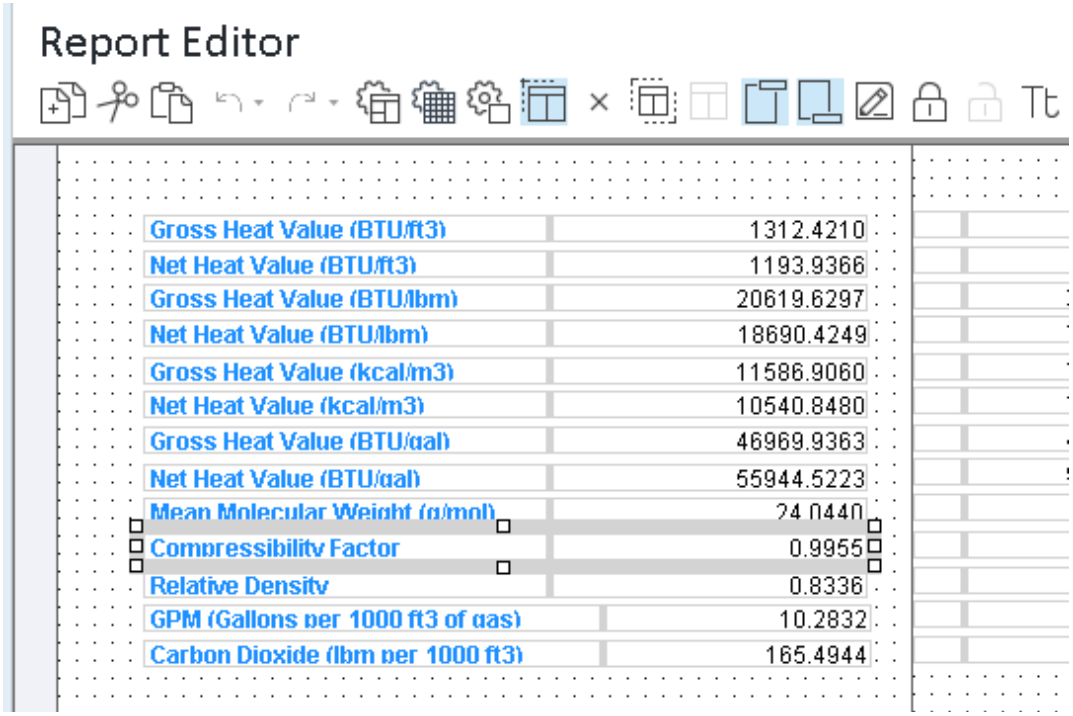


Figure 12. Report table

4 Right-click on **Compressibility Factor** and then select **Properties**.

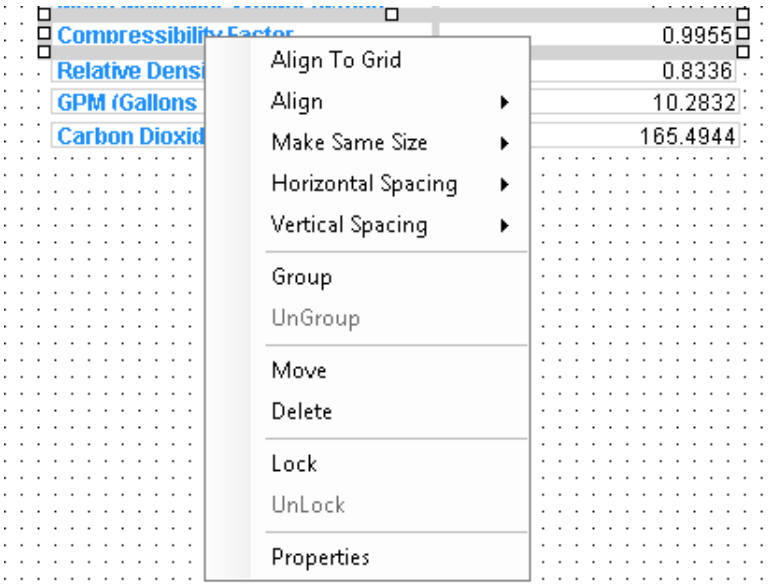


Figure 13. Report properties selector

This brings up the following screen.

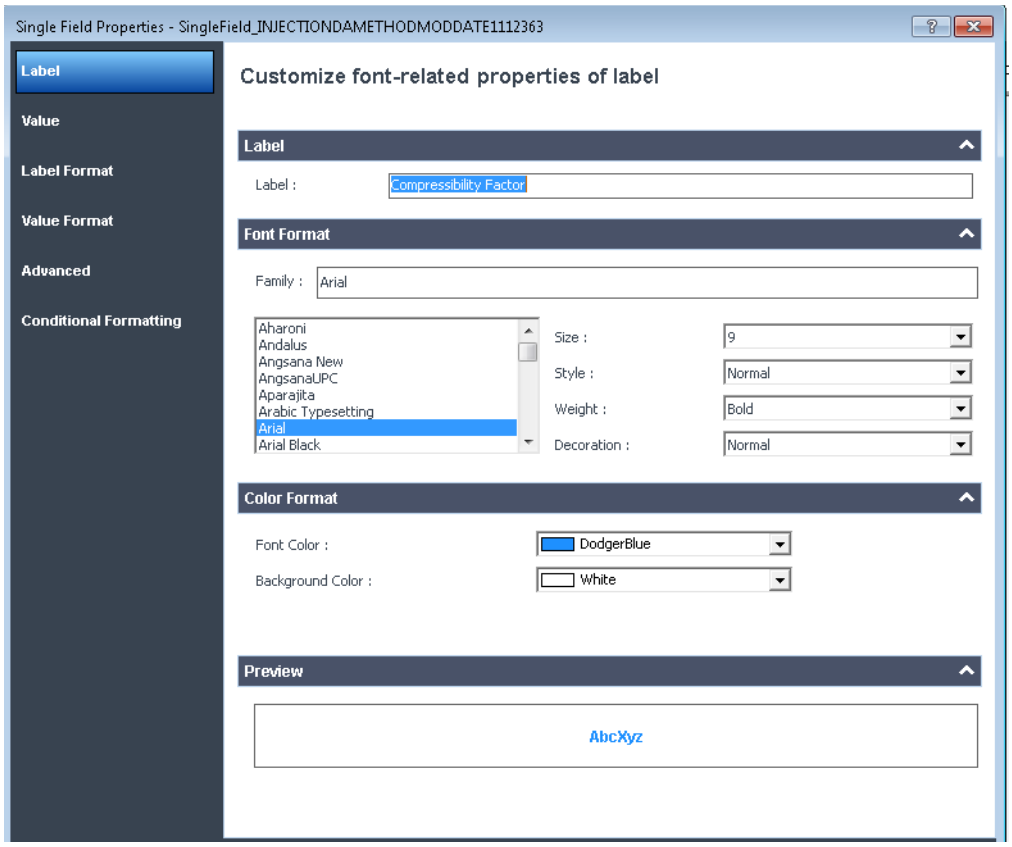


Figure 14. Single Field Properties

5 Change the **Label** to Factor de compresibilidad.

Figure 15. Report Label

6 Save the report template as a new report template.

7 Select **Preview** and click **Refresh Preview** to view the change. In this example, **Figure 16**, the Font color was also changed.

Real Gas Values

	Dry	Saturated
Gross Heat Value (BTU/ft3)	1312.4210	1290.9479
Net Heat Value (BTU/ft3)	1193.9366	1173.5998
Gross Heat Value (BTU/lbm)	20619.6297	20362.9181
Net Heat Value (BTU/lbm)	18690.4249	18445.1238
Gross Heat Value (kcal/m3)	11586.9060	11397.3269
Net Heat Value (kcal/m3)	10540.8480	10361.3016
Gross Heat Value (BTU/gal)	46969.9363	46324.7293
Net Heat Value (BTU/gal)	55944.5223	54991.5973
Mean Molecular Weight (g/mol)	24.0440	23.9389
Factor de compresibilidad	0.9955	0.9950
Relative Density	0.8336	0.8303
GPM (Gallons per 1000 ft3 of gas)	10.2832	10.1081
Carbon Dioxide (lbm per 1000 ft3)	165.4944	162.6755

Figure 16. Report name change

The new report template can now be used in the method by changing the selection of the Report template to the newly saved template.

Changing a Default Constants File Used During Method Update

The same approach can be used to use a modified constants file in method update. To do so, put your new constant files in the **Bin** directory of your DA installation (by default it is: C:\Program Files (x86)\Agilent Technologies\OpenLab Data Analysis\Bin).

To get a version of these files, you can use the web browser interface of your OpenLab Data Store to download them. In the OpenLab Data Store they will be stored in the method folder of your project and named similar to the following example: Metric_Constants_15_15_2015_02_03_17_2225276.txt.

These constant files are text (tab delimited) formatted.

To change them:

1 Open the .txt file in Microsoft Excel.

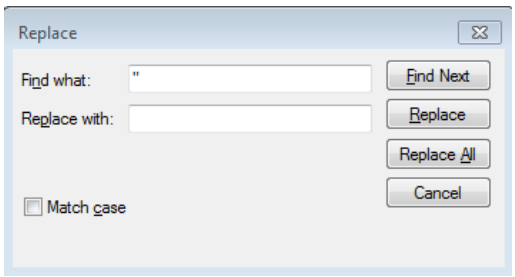
2 Change the values, and save the file as a *.txt file. In **Save as type**, choose **Text** (tab delimited) (*.txt).

3 When this file is saved, the compound names with commas are saved with quote marks, as shown in **Figure 17**.

```
n-heptane          7       16      100.2019        0.9948  0.0951  5502.6  2
methylcyclohexane          7       14      98.188  0.9958  0.0169054       5
"1,1,3-trimethylcyclopentane"      8       16      112.215 0.9957  0.017105
"2,2-dimethylhexane"       8       18      114.2285        0.9959  0.016702
"1,c-2-dimethylcyclopentane"       7       14      98.188  0.9953  0.017883
"2,5-dimethylhexane"       8       18      114.2285        0.9962  0.016080
"2,4-dimethylhexane"       8       18      114.2285        0.9963  0.015867
ethylcyclopentane          7       14      98.188  0.9958  0.0169054       5
```

Figure 17. Saved file opened in Notepad

Use the **Replace** function to remove the quotes for the file to be correctly formatted. An example file in Notepad after removing the quotation marks with the replace operation is shown in **Figure 17**.




```
n-heptane          7       16      100.2019        0.9948  0.0951  5502.6  2
methylcyclohexane          7       14      98.188  0.9958  0.0169054       5
1,1,3-trimethylcyclopentane        8       16      112.215 0.9957  0.0171055
2,2-dimethylhexane         8       18      114.2285        0.9959  0.0167029
1,c-2-dimethylcyclopentane         7       14      98.188  0.9953  0.0178834
```

Figure 18. Replace function

4 Rename the constants file and upload it to the OpenLab Data Store, once the file is modified. It will need to be uploaded to the method directory of the correct project.

5 View the **Custom Calculator** and change the **Constants path** for one the custom calculation listed.

6 The renamed file could be used by now saving the custom calculation file.

7 If this constants file is to be used as the default constants file, it has to be named as follows:

- FPS_Constants.txt-template
- Metric_Constants.txt-template
- ISO_6976_2016_Constants.txt-template

8 Click **Check file**:

- If the constants file is correctly formatted, there will be a message **Success File was successfully checked**.
- If the constants file is incorrectly formatted, **Check File** will generate **Constant file** (name of file) is not correctly formatted.

If you need to restore the original constant file, rename or remove the constant file from the Bin directory. When this is done, the Add-on will use the embedded constant file.

For example, ASTM 3588 in the Properties of Natural Gas Components table at 60°F and 14.696 psia gives values for Molar Mass, Molar Mass Ratio, Ideal Gross Heating Value (in kJ/mol, Btu/lbm, and Btu/ft3), the Ideal Net Heating Value (in kJ/mol, Btu/lbm, and Btu/ft3), and the Summation Factor. The table includes values for Butanes (ave), Pentanes (ave), Hexanes (ave), Butenes (ave), and Pentenes (ave). Pentenes (ave) could be added to a FPS constants file by opening the file in Excel adding Pentenes (ave) as the compound name and then values for the Molecular weight (MW), the summation factor (sum), the Gross and Net Heating values (BTU/ft3 and BTU/lb). The Gross and Net Heating Values (BTU/gal) needs to entered as 0 since the average liquid density is not given. The compressibility should be calculated from the summation factor and the Molar Ratio is entered in the table as SpecGrav.

	C	H	MW	Z (Compress)	sum	Gross BTU/ft^3	Gross BTU/lb	Gross BTU/gal
Pentenes_(ave)	5	10	70.134	calculate	0.060	3824	20691	0

Net BTU/ft^3	Net BTU/lb	Net BTU/gal	SpecGrav
3572	19328	0	2.4215

The values for ft3gas/lb, ft3/gal liq, Density liq, B.P. C, lbs/1000CF, Pc, Tc_F, Vc, and Acentric should be entered as zero values. Since lbs/1000CF can be calculated from the ideal gas law, this value can be calculated and used instead of zero in the table.

ft^{3}gas/lb	ft^3/gal liq	Density liq	B.P. C	lbs/1000CF	Pc	Tc_F	Vc	Acentric
0	0	0	0	calculate	0	0	0	0

9 Once the file is updated, follow the procedure outlined above to save and check the file. This file will be in the method folder under the project.

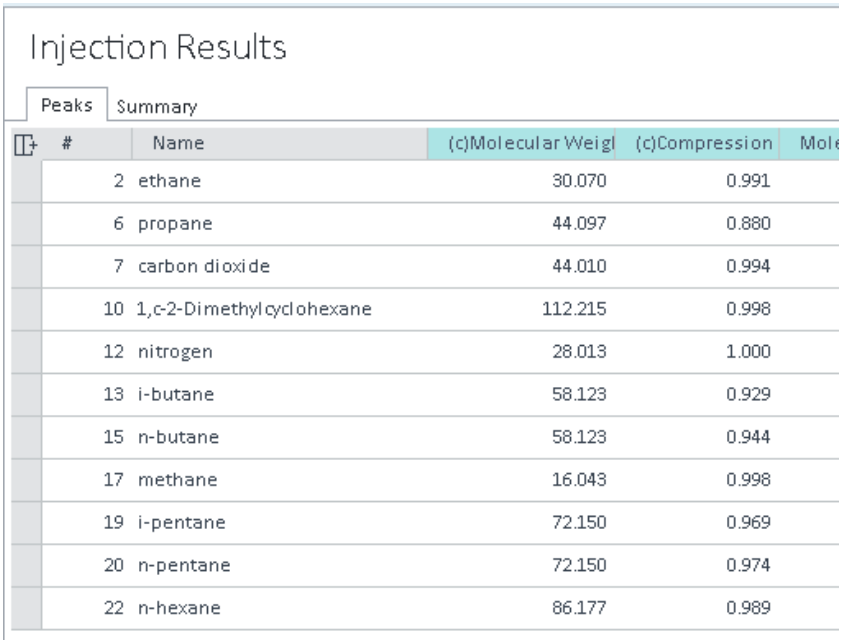
4 Troubleshooting

Empty Result

1 Check that all your peaks are identified correctly. To do so, you can check in the **Injection Results** pane the list of identified peak see **Figure 19**.

2 Check that for your identified compounds the expected constants have been found.

To do so, you can look in the **Injection Results**, the **(c)Compression factor** as example.



#	Name	(c)Molecular Weigl	(c)Compression	Mole
2	ethane	30.070	0.991	
6	propane	44.097	0.880	
7	carbon dioxide	44.010	0.994	
10	1,c-2-Dimethylcyclohexane	112.215	0.998	
12	nitrogen	28.013	1.000	
13	i-butane	58.123	0.929	
15	n-butane	58.123	0.944	
17	methane	16.043	0.998	
19	i-pentane	72.150	0.969	
20	n-pentane	72.150	0.974	
22	n-hexane	86.177	0.989	

Figure 19. Identified peak and related constant

If one of your compounds is not in the list of known compounds, you will not have any values for this compound. In **Figure 20**, the **Not existing compound** does not have a **(c)Compression factor** or a **(c)Molecular Weight** associated with it.

To solve this issue, you need either to use a valid name (see **“Appendix 1 - Compound Names”** on page 25), or provide a custom constant file (see **“Changing a Default Constants File Used During Method Update”** on page 18).

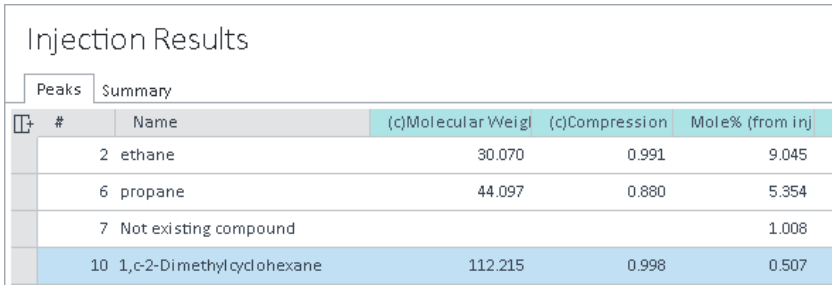


Figure 20. Not existing compound name

Inconsistent Results

Check that the calibration type selected in your NGA Add-on matches your method amount.

To do so, in the **Injection Results** window, you can check the **Amount**, **Mole % (from injection)**, **Weight % (from injection)**, or the **Volume % (from injection)** of your compound. See **Figure 21**.

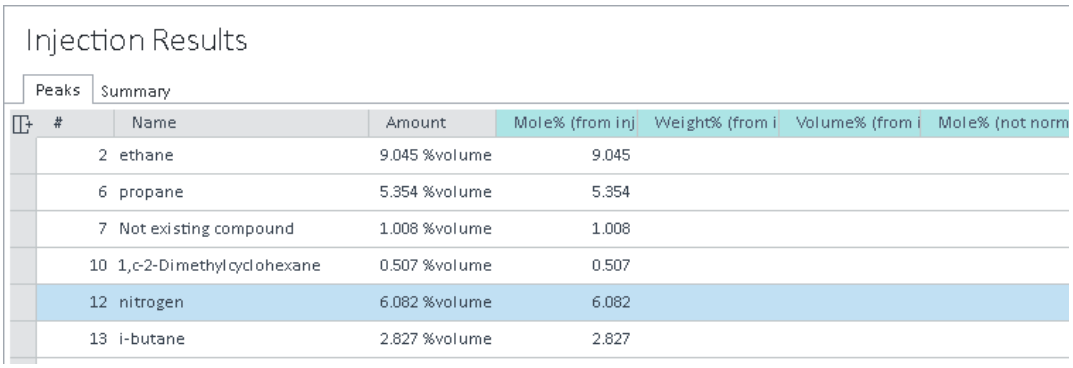
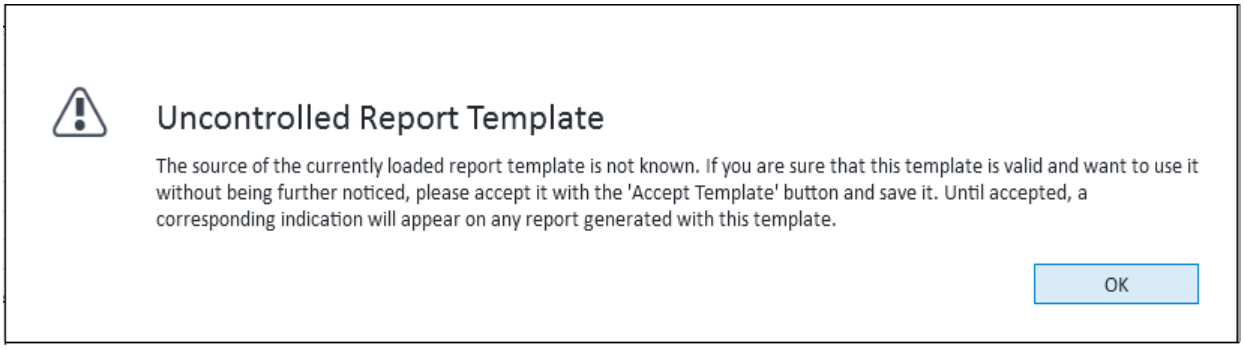


Figure 21. Amount and Mole % verification

Accept a Modified Template

If you use a report template that has been modified outside of OpenLab CDS 2.3, and has not yet been accepted, the **Uncontrolled Report Template** message is shown. See **Figure** .



Uncontrolled report template message

Your report will include an uncontrolled report **watermark**. See **Figure** .

Name	RT [min]	Area	Mole % (Dry)	Weight % (Dry)	Superior Heat Value (Dry) in BTU/ft3	Inferior Heat Value (Dry) in BTU/ft3
hydrogen	0.994	631.8	14.7202	0.8017	48.15	40.68
ethane	1.819	696.1	9.5755	7.7781	170.97	156.41
ethylene	2.116	72.0	0.9564	0.7248	15.44	14.46
propane	2.591	523.8	4.7853	5.7003	121.48	111.77
carbon dioxide	2.908	1892.8	8.4709	10.0710	0.00	0.00
propylene	3.692	103.5	0.9546	1.0851	22.47	21.01
nitrogen	3.696	13671.0	14.5298	10.9956	0.00	0.00
i-butane	4.075	1385.9	9.5781	15.0388	314.25	289.90
n-butane	4.286	680.5	4.7847	7.5126	157.48	145.35
methane	4.742	3289.8	4.8363	2.0959	49.28	44.37
carbon monoxide	5.013	4605.7	4.8422	3.6639	15.66	15.66
trans-2-butene	5.350	610.0	4.7782	7.2421	148.11	138.40
1-butene	5.477	1289.1	9.5585	14.4875	297.02	277.64
cis-2-butene	5.811	624.2	4.7710	7.2312	147.68	138.00
i-pentane	6.106	341.9	1.9078	3.7184	77.01	71.20
n-pentane	6.307	161.6	0.9506	1.8528	38.45	35.55

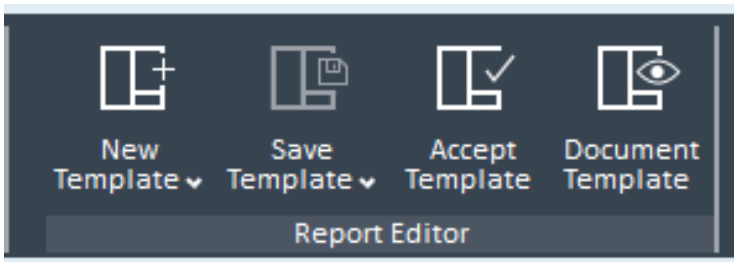
Uncontrolled report with watermark

Prerequisites

To perform the procedure as described, you need the privilege **Report Template > Validate Report Template.** Privileges are configured in the Control Panel.

1 Confirm the message with **OK**.

2 In the **Home** ribbon tab, click **Accept Template**. See **Figure** .



Home - Report Editor

3 Save the template.

Next time you load the template, it will be recognized as a validated template.

NOTE

As long as you do not click Accept Template, the message will be shown every time you load the report template. Even if you save the template under a new name, the application will keep showing the message until the template has been accepted.

All reports generated with an unaccepted template will show a corresponding warning symbol **watermark** in the background.

A Compound Names

The name of compounds defined in the FPS and Metric constant files are:

methane
ethane
propane
i-butane
n-butane
2,2-dimethylpropane
i-pentane
n-pentane
2,2-dimethylbutane
2,3-dimethylbutane
cyclopentane
2-methylpentane
3-methylpentane
n-hexane
2,2-dimethylpentane
methylcyclopentane
2,4-dimethylpentane
2,2,3-trimethylbutane
benzene
3,3-dimethylpentane
cyclohexane
2-methylhexane
2,3-dimethylpentane
1,1-dimethylcyclopentane
3-methylhexane
1,t-3-dimethylcyclopentane
1,c-3-dimethylcyclopentane
3-ethylpentane
1,t-2-dimethylcyclopentane
2,2,4-trimethylpentane
n-heptane
methylcyclohexane
1,1,3-trimethylcyclopentane
2,2-dimethylhexane
1,c-2-dimethylcyclopentane

2,5-dimethylhexane
2,4-dimethylhexane
ethylcyclopentane
2,2,3-trimethylpentane
1,t-2,c-4-trimethylcyclopentane
3,3-dimethylhexane
1,t-2,c-3-trimethylcyclopentane
2,3,4-trimethylpentane
2,3-dimethylhexane
toluene
1,1,2-trimethylcyclopentane
1,c-2,t-4-trimethylcyclopentane
2-methylheptane
4-methylheptane
3,4-dimethylhexane
3-methylheptane
3-ethylhexane
1,c-3-dimethylcyclohexane
1,c-2,t-3-trimethylcyclopentane
1,t-4-dimethylcyclohexane
2,2,5-trimethylhexane
1,1-dimethylcyclohexane
1-methyl-t-3-ethylcyciopentane
1-methyl-c-3-ethylcyciopentane
1-methyl-t-2-ethylcyclopentane
2,2,4-trimethylhexane
1-methyl-1-ethylcyclopentane
cycloheptane
n-octane
2,2,4,4-tetramethylpentane
1,t-3-dimethylcyclohexane
1,c-4-dimethylcyclohexane
1,c-2,c-3-trimethylcyclopentane
2,4,4-trimethylhexane
i-propylcyclopentane
2,3,5-trimethylhexane
2,2-dimethylheptane
2,4-dimethylheptane
1-ethyl-c-2-methylcyclopentane

2,2,3-trimethylhexane
1,c-2-dimethylcyclohexane
2,6-dimethylheptane
n-propylcyclopentane
1,c-3,c-5-trimethylcyclohexane
ethylcyclohexane
2,5-dimethylheptane
3,5-dimethylheptane
1,1,3-trimethylcyclohexane
2,3,3-trimethylhexane
3,3-dimethylheptane
1,1,4-trimethylcyclohexane
2,2,3,3-tetramethylpentane
ethylbenzene
2,3,4-trimethylhexane
1,t-2,t-4-trimethylcyclohexane
1,c-3,t-5-trimethylcyclohexane
m-xylene
p-xylene
3,4-dimethylheptane
2-methyloctane
4-methyloctane
3-methyloctane
1,t-2,c-3-trimethylcyclohexane
1,t-2,c-4-trimethylcyclohexane
o-xylene
1,1,2-trimethylcyclohexane
n-nonane
1,c-2,t-3-trimethylcyclohexane
1,c-2,c-3-trimethylcyclohexane
i-propylbenzene
i-propylcyclohexane
n-butylcyclopentane
propylcyclohexane
n-propylbenzene
m-ethyltoluene
p-ethyltoluene
4-methylnonane
5-methylnonane

1,3,5-trimethylbenzene
2-methylnonane
3-ethyloctane
3-methylnonane
o-ethyltoluene
1,2,4-trimethylbenzene
tert-butylbenzene
tert-butylcyclohexane
i-butylcyclohexane
n-decane
i-butylbenzene
sec-butylbenzene
1-methyl-3-isopropylbenzene
1,2,3-trimethylbenzene
1-methyl-4-isopropylbenzene
1-methyl-2-isopropylbenzene
n-butylcyclohexane
1,3-diethylbenzene
1-methyl-3-propylbenzene
1,2-diethylbenzene
n-butylbenzene
1-methyl-4-propylbenzene
1,4-diethylbenzene
1-methyl-2-propylbenzene
n-undecane
1,2,4,5-tetramethylbenzene
1,2,3,5-tetramethylbenzene
1,2,3,4-tetramethylbenzene
naphthalene
n-dodecane
2,3-dimethylheptane
1,c-2,t-4-trimethylcyclohexane
1,c-2,c-4-trimethylcyclohexane
i-butylcyclopentane
2,2-dimethyloctane
3,3-dimethyloctane
3,6-dimethyloctane
2,3-dimethyloctane
1,4-dimethyl-2-ethylbenzene

1,2-dimethyl-4-ethylbenzene
1,3-dimethyl-2-ethylbenzene
1,2-dimethyl-3-ethylbenzene
2-methylbutylbenzene
1-tert-butyl-2-methylbenzene
n-pentylbenzene
1-methyl-t-2-(4-methylpentyl)cyclopentane
1-tert-butyl-3,5-dimethylbenzene
1,2,4-triethylbenzene
1,3,5-triethylbenzene
n-hexylbenzene
n-tridecane
n-tetradecane
n-pentadecane
cyclopropane
nitrogen
oxygen
air
carbon dioxide
carbon monoxide
helium
hydrogen
hydrogen sulfide
water
ethylene
propylene
1-butene
cis-2-butene
trans-2-butene
2-methylpropene
1-pentene
propadiene
1,2-butadiene
1,3-butadiene
acetylene
methyl acetylene
cis-2-pentene
trans-2-pentene
2-methyl-2-butene

B ISO 6976:2016 Compound Names

The name of compounds defined in the ISO 67976:2016 constant file are:

methane
ethane
propane
n-butane 2-methylpropane (in place of i-butane)
n-pentane
2-methylbutane (in place of i-pentane)
2,2-dimethylpropane
n-hexane
2-methylpentane
3-methylpentane
2,2-dimethylbutane
2,3-dimethylbutane
n-heptane
n-octane
n-nonane
n-decane
n-undecane
n-dodecane
n-tridecane
n-tetradecane
n-pentadecane
ethene
propene
1-butene
Cis-2-butene
Trans -2-butene
2-methylpropene
1-pentene
Propadiene
1,2-butadiene
1,3-butadiene
Ethyne

cyclopentane
methylcyclopentane
ethylcyclopentane
cyclohexane
methylcyclohexane
ethylcyclohexane
benzene
toluene
ethylbenzene
o-xylene
methanol
methanethiol
hydrogen
water
hydrogen sulfide
ammonia
hydrogen cyanide
carbon monoxide
carbonyl sulfide
carbon disulfide
helium
neon
argon
nitrogen
oxygen
carbon dioxide
sulfur dioxide

www.agilent.com

Second edition, June 2021

../Graphics/AcceptTemplateRibbon.png @ 75 dpi 25
../Graphics/DownArrow.png @ 175 dpi 10
../Graphics/DownArrow.png @ 175 dpi 11
../Graphics/DownArrow.png @ 175 dpi 9
../Graphics/image1.png @ 150 dpi 7
../Graphics/image10.png @ 200 dpi 12
../Graphics/image11.png @ 200 dpi 13
../Graphics/image12.png @ 300 dpi 14
../Graphics/image13.png @ 150 dpi 15
../Graphics/image14.png @ 150 dpi 15
../Graphics/image15.png @ 150 dpi 16
../Graphics/image16.png @ 150 dpi 16
../Graphics/image17.png @ 150 dpi 17
../Graphics/image18.png @ 175 dpi 18
../Graphics/image19.png @ 150 dpi 18
../Graphics/image2.png @ 150 dpi 9
../Graphics/image20.png @ 175 dpi 18
../Graphics/image21.png @ 150 dpi 21
../Graphics/image22.png @ 150 dpi 22
../Graphics/image23.png @ 150 dpi 23
../Graphics/image3.png @ 150 dpi 10
../Graphics/image4.png @ 110 dpi 10
../Graphics/image5.png @ 150 dpi 11
../Graphics/image6.png @ 150 dpi 11
../Graphics/image8.png @ 150 dpi 11
../Graphics/image9.png @ 150 dpi 12
../Graphics/RightArrow.png @ 175 dpi 11
../Graphics/RightArrow.png @ 175 dpi 9
../Graphics/select-computation-type.png @ 300 dpi 11
../Graphics/Template_Table_Watermarked.png @ 72 dpi 24
../Graphics/Uncontrolled_Report_Template_fixed.png @ 150 dpi 24